

Isobutyl nitrite
542-56-3 | DTXSID3020750

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	1.14	0.85	1.12	0.83	1.23

Model Results

Predicted value: 1.50e-12 cm³/molecule*sec

Global applicability domain: Inside

Local applicability domain index: 6.52e-01

Confidence level: 8.04e-01

Nearest Neighbors from the Training Set

Image not found

N-Butylnitrite

Measured: 2.72e-12

Predicted: 1.86e-12

Image not found

1-Nitrobutane

Measured: 1.50e-12

Predicted: 1.21e-12

Image not found

Isobutyl nitrate

Measured: 9.20e-13

Predicted: 1.33e-12

Image not found

Butyl nitrate

Measured: 1.71e-12

Predicted: 1.60e-12

Image not found

1-Nitropropane

Measured: 4.40e-13

Predicted: 5.94e-13